

The structure of superheavy elements newly discovered in the reaction of ^{86}Kr with ^{208}Pb

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The structure of superheavy elements newly discovered in the $^{208}\text{Pb}(^{86}\text{Kr},n)$ reaction at Berkeley is systematically studied in the Relativistic Mean Field (RMF) approach. It is shown that various usually employed RMF forces, which give fair description of normal stable nuclei, give quite different predictions for superheavy elements. Among the effective forces we tested, TM1 is found to be the good candidate to describe superheavy elements. The binding energies of the $^{293}118$ nucleus and its α -decay daughter nuclei obtained using TM1 agree with those of FRDM within 2 MeV. Similar conclusion that TM1 is the good interaction is also drawn from the calculated binding energies for Pb isotopes with the Relativistic Continuum Hartree Bogoliubov (RCHB) theory. Using the pairing gaps obtained from RCHB, RMF calculations with pairing and deformation are carried out for the structure of superheavy elements. The binding energy, shape, single particle levels, and the Q values of the α -decay Q_α are discussed, and it is shown that both pairing correlation and deformation are essential to properly understand the structure of superheavy elements. A good agreement is obtained with exper-

imental data on Q_α .

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I. INTRODUCTION

Following the discovery of α -decay isotopes of Elements $Z = 110, 111$, and 112 at GSI [1–3], an isotope of the Element 118 , $^{293}118$, and several its α -decay daughter nuclei were announced to have been discovered at Berkeley Lab’s 88-Inch Cyclotron with the newly constructed Berkeley Gas-filled Separator by bombarding lead target with an intense beam of krypton ions of 449 MeV [4]. The sequence of decay events is consistent with the long-standing theoretical prediction that there exists an “island of stability” around 114 protons and 184 neutrons and activates once again the study of superheavy elements.

The study of superheavy elements has been a hot topic for the last two decades. Recent works on the collisions, structure and stability of Heavy and Superheavy Elements can be found in Refs. [5–11]. In a recent paper, Smolanczuk claimed that the reaction $^{208}\text{Pb}(^{86}\text{Kr}, n)$ should have a particularly favorable production rate [12]. This motivated the experiment at Berkeley. According to the authors, the synthesized superheavy element $^{293}118$ decays by emitting an alpha particle within less than a millisecond, leaving behind the isotope of element 116 with mass number 289 . This daughter nucleus is also radioactive, alpha-decaying to an isotope of element 114 . The chain of successive alpha decays continues until element 106 .

Smolanczuk discussed also the properties of superheavy elements in this mass region under the constraint of a spherical shape based on a macroscopic-microscopic approach [13]. In contrast to his approach, here we study the structure of superheavy element $^{293}118$ and of the daughter nuclei in the sequence of α decays in the Relativistic Mean Field (RMF) theory. The effects of deformation and pairing correlation will be taken into account. The pairing gaps for deformed RMF calculations are taken from the Relativistic Continuum Hartree

Bogoliubov (RCHB) theory [14], which is an extension of the Relativistic Mean Field and the Bogoliubov transformation in the coordinate representation [15]. As the spin-orbit splitting which governs the shell structure and magic number is naturally obtained in the RMF theory, we expect that the structure of superheavy elements can be understood properly once the deformation and pairing correlation are taken into account. We investigate the binding energy, deformation, the Q -values of the alpha decay, the effect of pairing correlation, shell structure, and the structure of single particle levels for protons and neutrons.

The paper is organized as follows. In sect.II, we present the results of RMF calculations without pairing correlation for several standard forces, which give fair description of normal stable nuclei. We thus discuss the appropriate force to describe superheavy elements. In sect.III the RCHB theory is used to investigate the pairing correlation in these superheavy elements. The RCHB provides not only a unified description of mean field and pairing correlation but also a proper description for the continuum and the coupling between the bound state and the continuum [14]. We then perform in sect.IV the study by a deformed RMF+BCS approach using the pairing gaps supplied by RCHB. We summarize the paper in sect.V.

II. EXAMINATION OF VARIOUS RMF PARAMETER SETS

There are many parameter sets for RMF calculations, which provide nearly equal quality of description for stable nuclei. Therefore, we wish to find at first which effective force in RMF is more suitable to describe superheavy elements. As claimed in Ref. [11] the results are strongly interaction dependent. For this purpose we perform RMF calculations that include deformation but ignore pairing correlation with different effective forces. The details of the method can be found in Ref. [16].

Table I compares the binding energies E of superheavy element $^{293}118$ and its α decay daughter nuclei calculated with effective forces TM1 [17], NL1, NL3 and NLSH. For comparison, the results of the phenomenological FRDM calculations are given in the last column [18].

The results of TM1 are nearly the same as those of FRDM for $^{265}_{104}$, $^{269}_{106}$, $^{273}_{108}$, $^{277}_{110}$, and $^{281}_{112}$. They are within 1 MeV from each other. The difference between TM1 and FRDM results gets larger for $^{285}_{114}$, $^{289}_{116}$ and $^{293}_{118}$, but is still smaller than 3 MeV. Though there are differences of several MeV, NL1 and NLSH give similar results as TM1. The NL3 parameter set, on the other hand, gives a difference of about 50 MeV from the other calculations.

One important difference between the RMF calculations with TM1 and FRDM is that the additional gain of the binding energy when one moves from $^{281}_{112}$ to $^{285}_{114}$ is much less in the RMF calculations. In other words, $Z=114$ has a weaker meaning as a magic number in the RMF calculations. Though, strictly speaking, it may not be adequate, let us call this effect as the change of the shell structure or of the magic number property at $Z=112$. As we see shortly, a similar effect appears in the Z dependence of the nuclear shape. This effect eventually plays an important role in reproducing the qualitative trend of the experimental data on the atomic number dependence of Q_α .

TABLE I. The binding energy E of the superheavy element $^{293}_{118}$ and of its α decay daughter nuclei calculated in the RMF theory with different effective interactions TM1, NL1, NL3, and NLSH. The prediction of FRDM is also given in the last column.

$^A_Z N$	TM1	NL1	NL3	NLSH	FRDM
$^{265}_{104}_{161}$	1949.2	1953.0	1912.5	1950.5	1950.0
$^{269}_{106}_{163}$	1970.2	1974.1	1932.0	1977.5	1970.5
$^{273}_{108}_{165}$	1990.2	1992.8	1950.9	1997.9	1989.4
$^{277}_{110}_{167}$	2007.9	2010.5	1968.2	2016.1	2007.0
$^{281}_{112}_{169}$	2026.2	2029.8	1986.2	2034.7	2025.2
$^{285}_{114}_{171}$	2041.3	2051.8	2003.0	2048.7	2044.1
$^{289}_{116}_{173}$	2058.2	2068.7	2014.2	2065.6	2061.1
$^{293}_{118}_{175}$	2074.7	2088.9	2028.7	2080.5	2077.2

Similar trend concerning the mutual comparison of different forces appears also in Table II, where the Q-values of α decay sequence $Q_\alpha = E(^4He) + E(Z - 2, N - 2) - E(Z, N)$ (MeV) are shown. The Q-values given by TM1 and FRDM are quite similar except for $^{285}114$, where the difference is 3.8 MeV. This large difference is connected with the change of the shell structure mentioned above.

TABLE II. The Q-values of α decay for superheavy element $^{293}118$ and its α decay daughter nuclei. We used the experimental value for the binding energy of the α particle.

A_ZN	<i>TM1</i>	<i>NL1</i>	<i>NL3</i>	<i>NLSH</i>	<i>FRDM</i>
$^{269}_{106}163$	8.3	7.2	8.8	1.3	7.8
$^{273}_{108}165$	8.3	9.6	9.4	7.9	9.4
$^{277}_{110}167$	10.6	10.6	11.0	10.1	10.7
$^{281}_{112}169$	10.0	9.0	10.3	9.7	10.1
$^{285}_{114}171$	13.2	6.3	11.5	14.3	9.4
$^{289}_{116}173$	11.4	11.4	17.1	11.4	11.3
$^{293}_{118}175$	11.8	8.1	13.8	13.4	12.2

Table III shows the corresponding deformation parameter β in the ground state. TM1 predicts a stable prolate deformation $\beta \sim 0.2$ for all the nuclei listed in the table, taking the minimum at $^{281}112$. NL3 and NLSH give similar results as TM1, but the minimum deformation is shifted to $^{285}114$ for NL3. The NL1 predicts a spherical shape for $^{293}118$, while FRDM almost spherical shape for $^{277}110$, $^{281}112$, $^{285}114$, $^{289}116$ and $^{293}118$. The shift of the atomic number, where the deformation becomes minimum, from $Z=114$ to 112 is what we already mentioned as an evidence of the change of the shell structure.

TABLE III. The deformation β of the superheavy element $^{293}118$ and its α decay daughter nuclei calculated with different effective interactions TM1, NL1, NL3, and NLSH. The prediction of FRDM is also given in the last column.

$^A Z_N$	<i>TM1</i>	<i>NL1</i>	<i>NL3</i>	<i>NLSH</i>	<i>FRDM</i>
$^{265}104_{161}$	0.2656	0.2687	0.2685	0.2513	0.222
$^{269}106_{163}$	0.2059	0.2576	0.2479	0.2073	0.221
$^{273}108_{165}$	0.2021	0.2438	0.2032	0.2068	0.173
$^{277}110_{167}$	0.1857	0.2279	0.1865	0.1914	0.089
$^{281}112_{169}$	0.1681	0.2072	0.1683	0.1741	-.096
$^{285}114_{171}$	0.2118	0.1593	0.1606	0.2316	0.080
$^{289}116_{173}$	0.2373	0.1548	0.2163	0.2566	0.081
$^{293}118_{175}$	0.2340	0.0600	0.2402	0.2946	0.080

Table IV compares the corresponding charge-radii R_c . In contrast to the big difference seen in the binding energy, the charge-radii R_c for different forces lie within 1% from each other.

TABLE IV. Comparison of the charge-radii R_c of superheavy element $^{293}118$ and its α decay daughter nuclei calculated with different parameter sets.

AZ_N	$TM1$	$NL1$	$NL3$	$NLSH$
$^{269}106_{163}$	6.146	6.153	6.177	6.104
$^{273}108_{165}$	6.174	6.176	6.197	6.134
$^{277}110_{167}$	6.197	6.203	6.220	6.158
$^{281}112_{169}$	6.226	6.228	6.247	6.188
$^{285}114_{171}$	6.282	6.248	6.275	6.250
$^{289}116_{173}$	6.332	6.272	6.340	6.303
$^{293}118_{175}$	6.360	6.276	6.392	6.355

III. PAIRING CORRELATION IN SUPERHEAVY ELEMENTS: DESCRIPTION BY RCHB

In this section we study the effects of pairing correlation in superheavy element $^{293}118$ and its α decay daughter nuclei by using the self-consistent and fully microscopic RCHB theory [14] under the constraint of a spherical shape. With the pairing gap obtained from RCHB, a self-consistent and more complete RMF calculation with both pairing correlation and deformation will be carried out in the next section.

Before applying the RCHB theory to newly discovered superheavy elements, we examine once again which effective force is the most suitable to describe superheavy elements. For this purpose, we use lead isotopes as test cases.

TABLE V. Comparison of the binding energies E of Pb isotopes calculated in RCHB theory with 4 different parameter sets with experimental data. The last four columns are the root mean square neutron, proton, matter and charge radii calculated with the TM1 parameter set.

A(Pb)	Exp.[MeV]	TM1	NL1	NL3	NLSH	R_N	R_P	R_M	R_C
202	1592.20	1592.91	1596.60	1565.43	1596.00	5.629	5.420	5.545	5.479
204	1607.52	1609.18	1611.35	1580.36	1611.35	5.656	5.429	5.566	5.487
206	1623.40	1623.78	1625.73	1594.77	1626.11	5.683	5.437	5.586	5.495
208	1636.45	1637.76	1639.72	1608.56	1639.99	5.713	5.447	5.609	5.505
210	1645.57	1646.92	1646.78	1618.04	1648.34	5.743	5.467	5.636	5.525
212	1654.52	1655.73	1653.57	1626.97	1656.43	5.772	5.486	5.663	5.544

The binding energies of six Pb isotopes calculated by RCHB with 4 different effective forces are compared with experimental data in Table V . Although all the calculations except for NL3 well reproduce the experimental binding energies of the Pb isotopes, TM1 gives the best reproduction of the data. Therefore we expect that the RMF calculations with TM1 and pairing correlation will give a satisfactory description of superheavy elements. The *rms* radii for neutron R_N , proton R_P , matter R_M , and charge radii R_C calculated by RMF with TM1 are given in the last four columns in Table V.

TABLE VI. The binding energy E , one neutron separation energy S_n , the Q value for the α decay Q_α , matter and charge *rms* radii R_m and R_c , neutron and proton pairing gaps in RCHB with TM1 for the superheavy element $^{293}118$ and its α decay daughter nuclei. The results for ^{86}Kr , ^{208}Pb and $^{294}118$ are also given.

$^A Z_N$	E	S_n	Q_α	R_m	R_c	Δ_n/Δ_p
$^{86}\text{Kr}_{50}$	750.2			4.221	4.182	-0.010/-1.304
$^{208}\text{Pb}_{126}$	1637.6			5.649	5.541	-0.000/-0.000
$^{265}104_{161}$	1944.4			6.175	6.099	-0.622/-1.173
$^{269}106_{163}$	1965.6	4.9	7.1	6.202	6.131	-0.421/-1.146
$^{273}108_{165}$	1986.8	5.9	7.1	6.228	6.160	-0.283/-1.133
$^{277}110_{167}$	2007.2	5.5	7.9	6.255	6.189	-0.380/-1.092
$^{281}112_{169}$	2027.1	6.3	8.4	6.281	6.218	-0.338/-1.030
$^{285}114_{171}$	2046.8	6.6	8.6	6.308	6.247	-0.030/-0.948
$^{289}116_{173}$	2065.2	5.8	9.9	6.333	6.273	-0.013/-0.841
$^{293}118_{175}$	2082.1	5.9	11.5	6.356	6.296	-0.315/-0.696
$^{294}118_{176}$	2088.8	6.7		6.364	6.299	-0.442/-0.702

We have then calculated the binding energy E , one neutron separation energy S_n , the Q value for the α decay Q_α , matter and charge *rms* radii R_m and R_c , neutron and proton pairing gaps for superheavy elements in the RCHB with TM1. The results are shown in Table VI. The matter *rms* radius R_m is larger than the charge *rms* radius R_c for all nuclei due to the neutron excess. The Q value of the α decay increases monotonically with Z . The proton pairing gap parameter is around 1 MeV, while the neutron pairing gap parameter is relatively small due to blocking effects. The calculation for ^{86}Kr , ^{208}Pb and $^{294}118$ are also given for reference to understand the fusion barrier to synthesize the element $^{294}118$.

In Figs.1 and 2, the single particle levels in the canonical basis for neutrons and protons in $^{292}118$ are given, respectively. In order to avoid the irregularity due to the blocking effect, we give the single particle levels in $^{292}118$ instead of $^{293}118$. The Fermi surface for neutrons and protons is given in each figure by the dashed line. The potential is the sum of the vector and scalar potentials. Fig.1 indicates that, after the sub-closed shell at $N = 164$, the next closed or sub-closed shells occur at $N = 198$ and $N = 210$. For the proton case, closed or sub-closed shells occur at $Z = 106$, $Z = 114$ and $Z = 120$.

The Fermi level for protons in $^{293}118$ is at $\lambda = -1.916$ MeV, while that for neutrons at $\lambda = -6.304$ MeV. Although the Fermi level for protons is very close to the continuum, the wave functions of all the protons are well localized in a small region because of the Coulomb barrier.

Figs.3 and 4 show the change of the single particle neutron and proton levels near the Fermi surface along the α -decay chain from $^{293}118$. Similarly to Figs.1 and 2, we give the single particle levels for the neighboring even-even nuclei in order to avoid the irregularity due to the blocking effect. Adding an α particle always raises the proton single particle levels and lowers the neutron single particle levels. There are distinct gaps of about 2 MeV at $N = 164$ and 172 and of about 3 MeV at $N = 198$ for neutrons.

The α -decay energy Q_α is shown in Fig.5 as a function of the atomic number along the decay chain from $^{293}118$. The observed data and the prediction of FRDM are also included, where the former are taken from Fig.4 in [4]. Compared with the data, RCHB calculations give systematically too small Q_α . This reflects the deformation effect which is ignored in

the present RCHB calculations. The Q_α calculated in the RMF calculations neglecting the pairing correlation but including the deformation (the open circles) is somewhat larger than that in RCHB but still smaller than the data for $Z < 108$ and fluctuates for larger Z showing a sharp peak at $Z = 114$. This contrasts to the result of FRDM, which also fluctuates, but shows a deep minimum at the same atomic number reflecting a sub-closed shell at $Z = 114$ in this model.

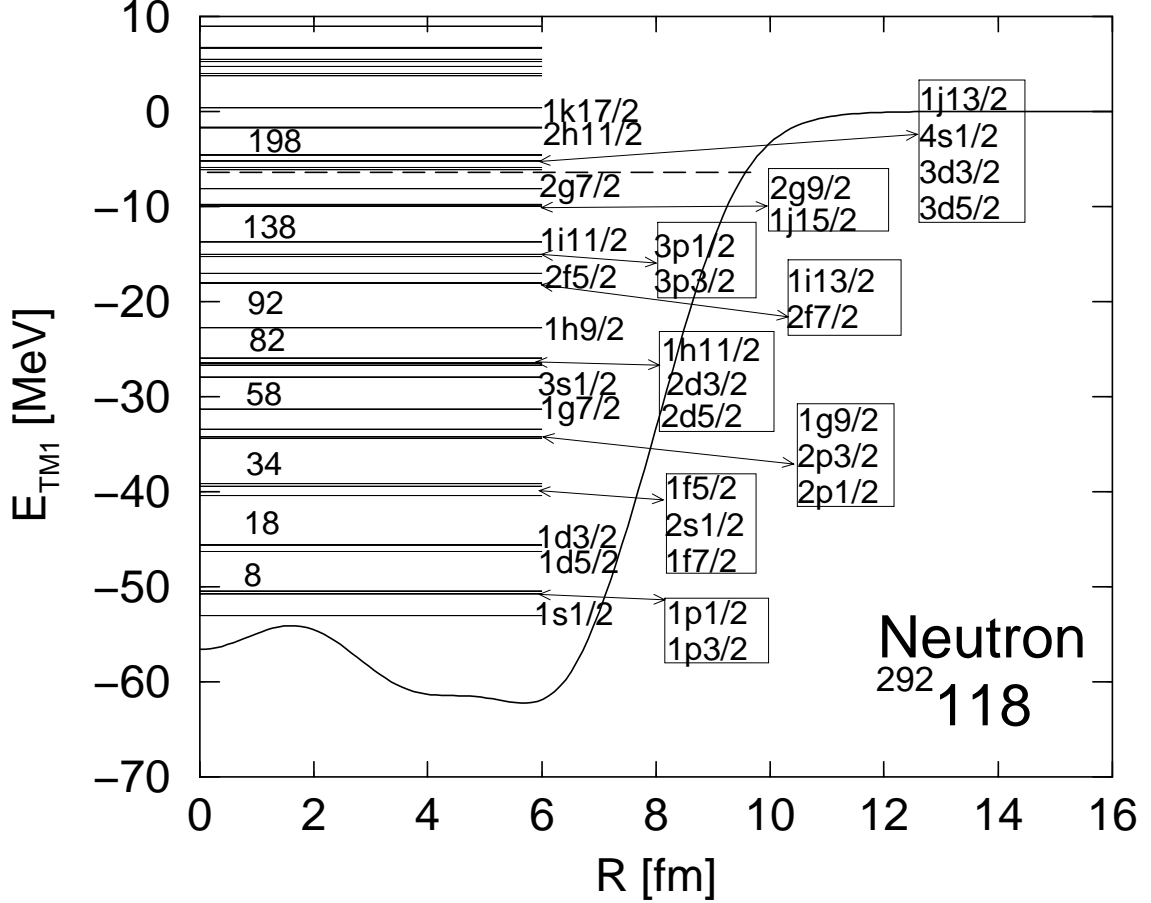


FIG. 1. The single particle levels in the canonical basis for neutrons in $^{292}_{118}$ calculated by RCHB with TM1. The neutron potential $V_V(r) + V_S(r)$ is represented by the solid line and the Fermi level by a dashed-line.

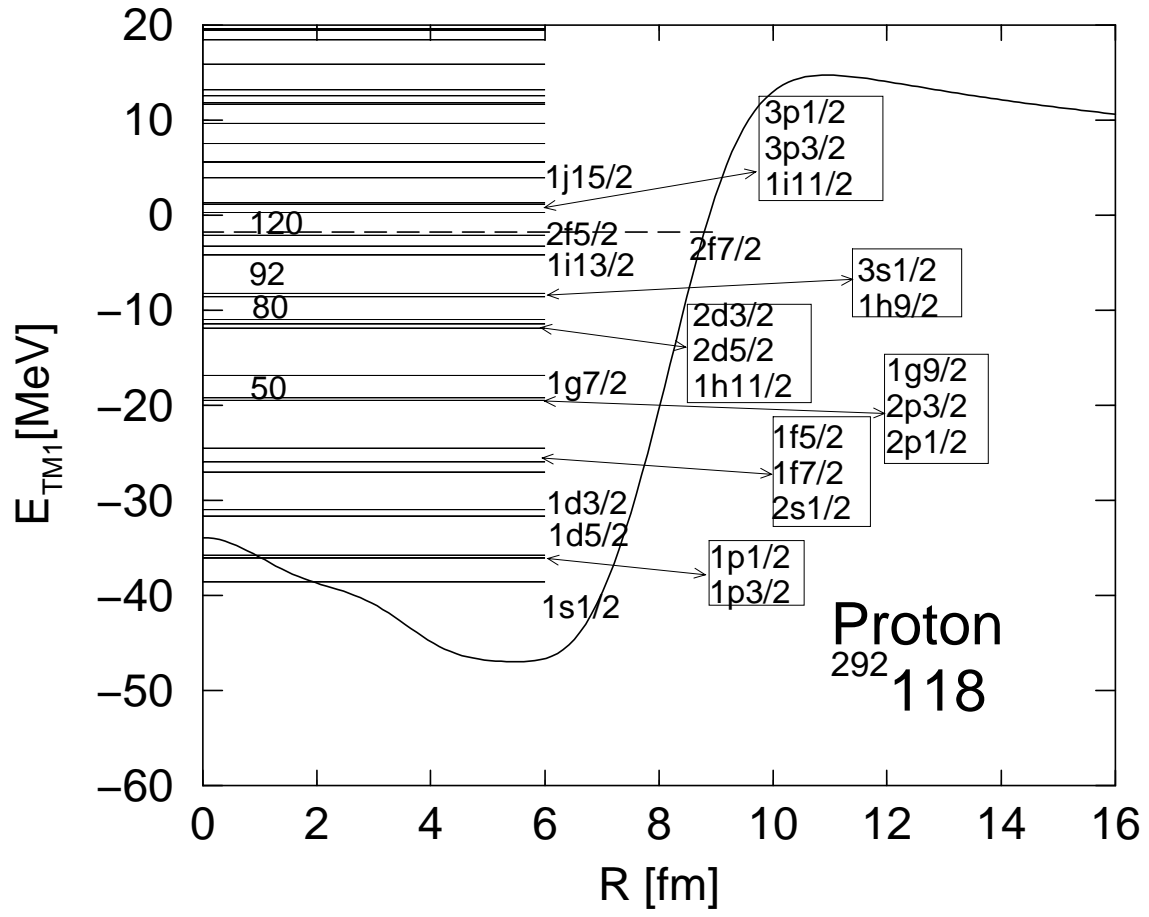


FIG. 2. The same as Fig.1, but for protons.

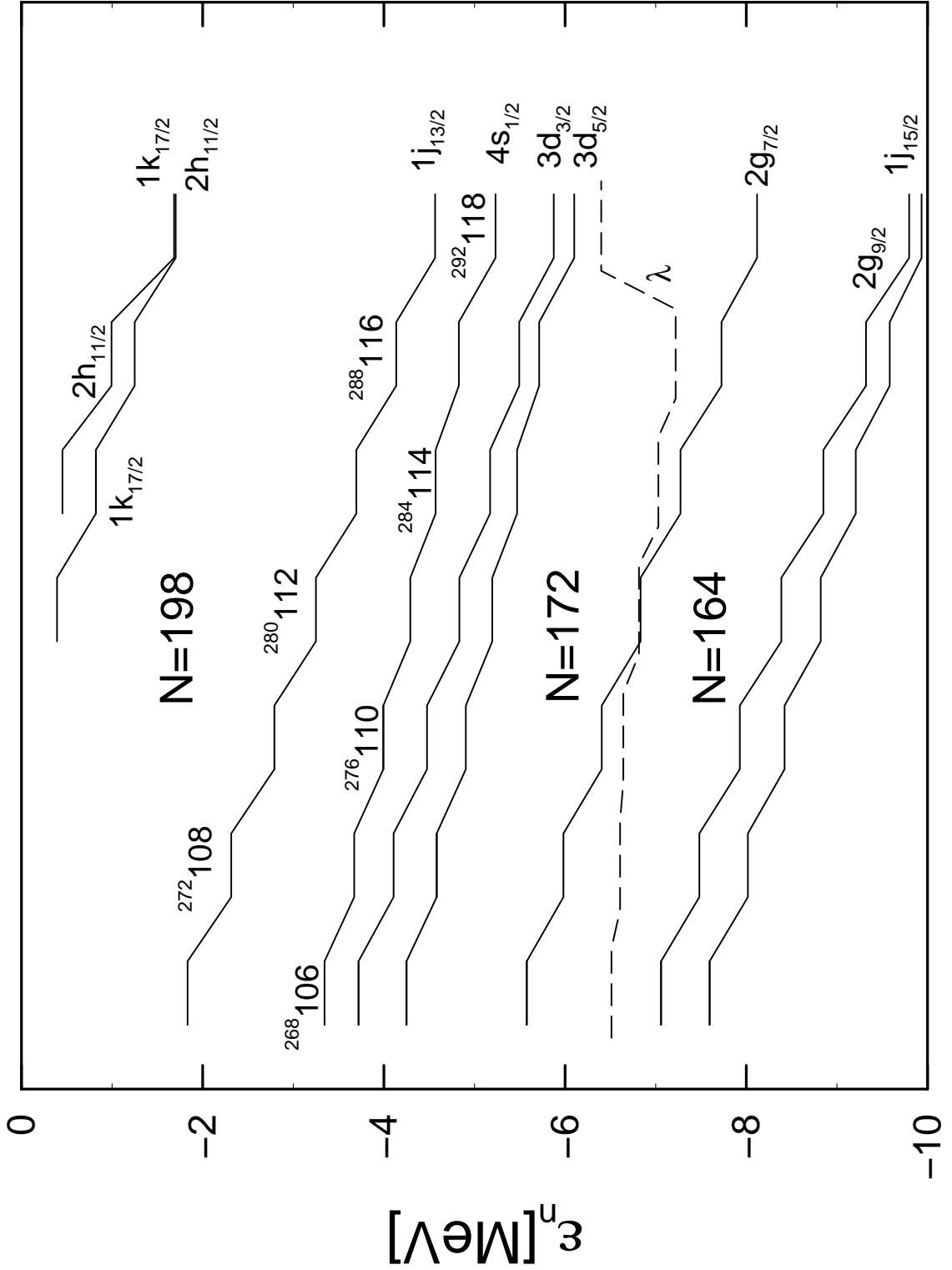


FIG. 3. The single particle levels for neutrons near the Fermi surface calculated in the RCHB with TM1. They are shown for the neighboring even-even nuclei to the superheavy elements in the α -decay chain from $^{293}\text{118}$.

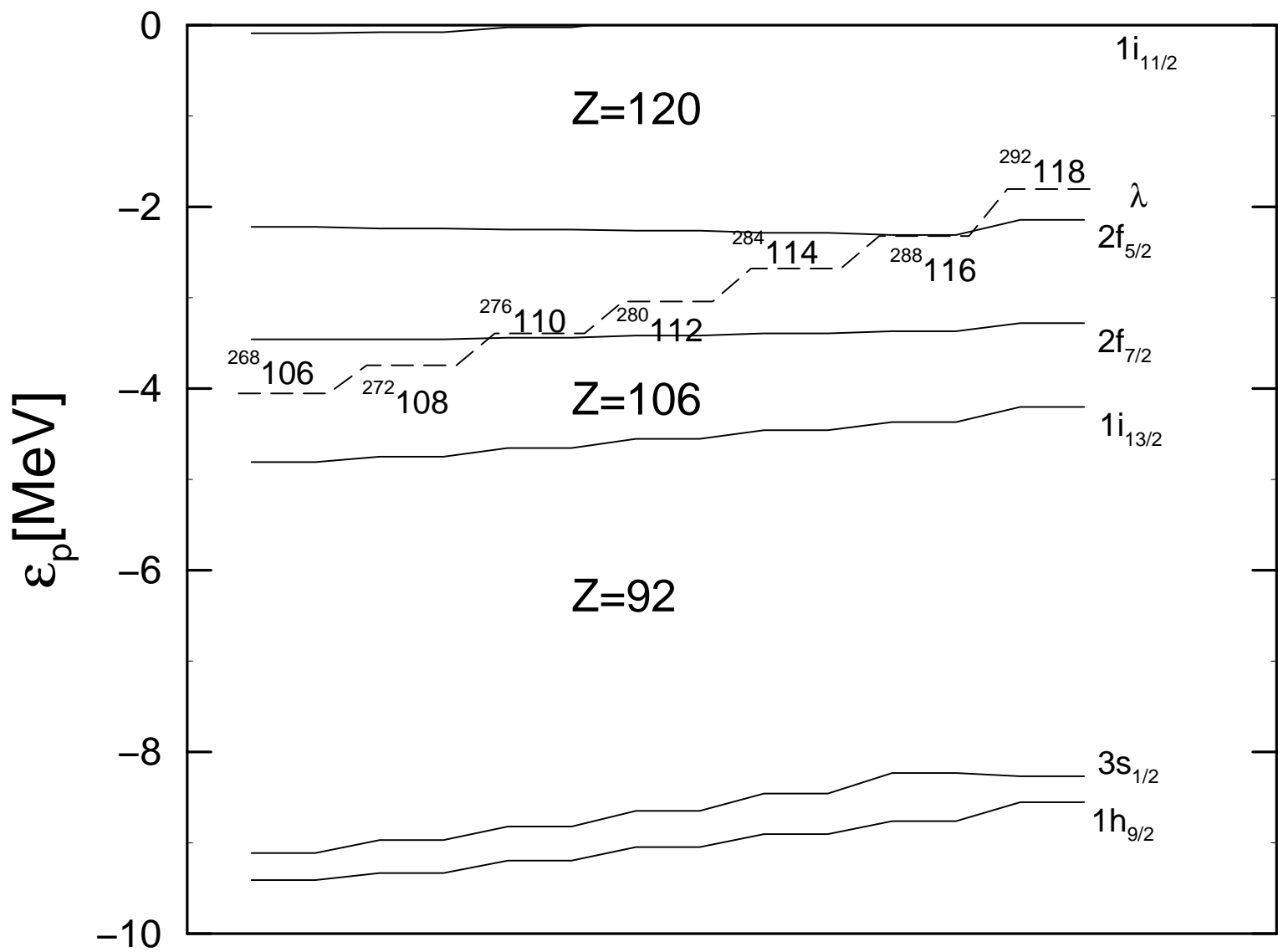


FIG. 4. The same as Fig.3, but for protons.

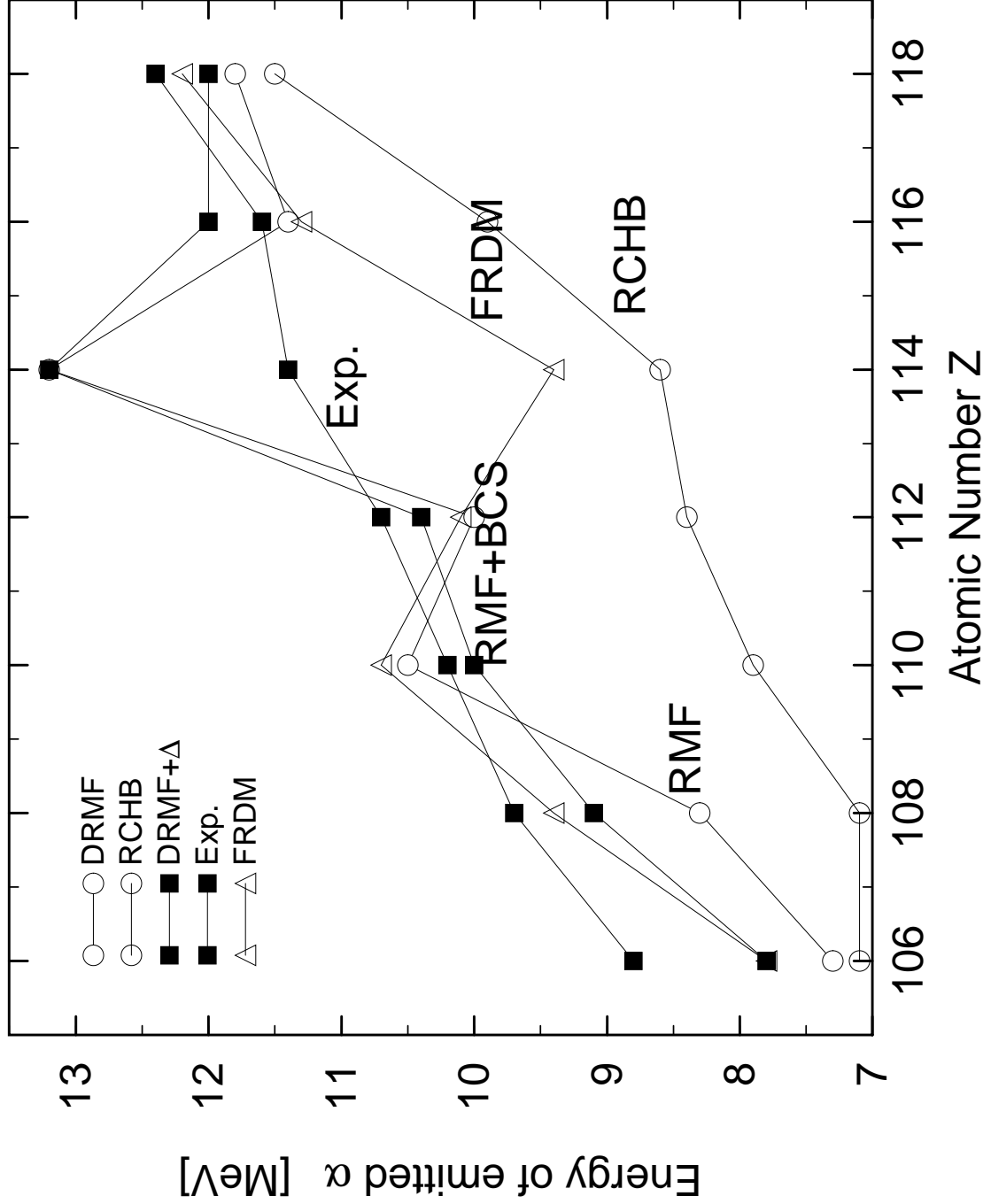


FIG. 5. Comparison of the theoretical α particle energies Q_α with the observed data.

IV. THE DESCRIPTION OF SUPERHEAVY ELEMENTS BY DRMF+BCS

Using the pairing gap from RCHB, we now perform the RMF calculations by including both deformation and pairing correlation. The results are given in Table VII for the binding

energy E , the α -particle energy, matter and charge radii, and the neutron, proton and matter deformation parameters. The calculated binding energies for ^{86}Kr , ^{208}Pb and $^{294}118$ are also given. Each binding energy increases by 0.3 to 2 MeV with the pairing correlation, and can noticeably alter the atomic number dependence of Q_α .

We added the results of Q_α calculated by the DRMF+BCS in Fig.5. Comparing with RMF calculations, we observe that the theoretical Q_α becomes much closer to the experimental data by the inclusion of the pairing correlation. Only for $Z = 114$, the Q_α remains the same and has a difference of 2 MeV from the data. Interestingly, Q_α takes maximum at $Z = 114$ in DRMF+BCS in accord with the hump in the data, while the FRDM gives a minimum there.

TABLE VII. The binding energy E , α -decay Q value, matter and charge radii, and neutron, proton and matter deformation parameters calculated in the DRMF+BCS theory with TM1.

$^A Z_N$	E	Q_α	R_m	R_c	β_n	β_p	β
$^{86}\text{Kr}_{50}$	751.0		4.222	4.189	0.003	0.005	0.004
$^{208}\text{Pb}_{126}$	1636.8		5.650	5.544	0.000	0.0000	0.000
$^{265}104_{161}$	1951.4		6.206	6.117	0.212	0.210	0.211
$^{269}106_{163}$	1971.9	7.8	6.232	6.147	0.208	0.207	0.208
$^{273}108_{165}$	1991.1	9.1	6.256	6.175	0.197	0.197	0.197
$^{277}110_{167}$	2009.4	10.0	6.279	6.202	0.178	0.178	0.178
$^{281}112_{169}$	2027.3	10.4	6.302	6.228	0.164	0.164	0.164
$^{285}114_{171}$	2042.4	13.2	6.347	6.280	0.204	0.202	0.203
$^{289}116_{173}$	2058.7	12.0	6.390	6.328	0.227	0.228	0.227
$^{293}118_{175}$	2075.0	12.0	6.423	6.363	0.230	0.234	0.232
$^{294}118_{176}$	2081.3		6.429	6.365	0.224	0.229	0.226

V. SUMMARY

We made a systematic study of the structure of superheavy elements recently discovered at Berkeley Lab's 88-Inch Cyclotron by the reaction $^{86}\text{Kr} + ^{208}\text{Pb}$ at 449 MeV in the framework of Relativistic Mean Field (RMF) approach. We have shown that usually used various RMF forces, which provide fair description of normal stable nuclei, give quite different predictions for superheavy elements. Among them TM1 is found to be the good candidate to describe superheavy elements.

We have shown that the binding energy obtained from TM1 agrees with that of FRDM within a difference of 2 MeV. The same conclusion that TM1 is the good interaction has been drawn from the calculations of the binding energy of Pb isotopes using Relativistic Continuum Hartree Bogoliubov (RCHB) theory. However, neither the deformation nor the pairing correlation alone could explain the data of Q_α .

We then performed RMF calculations of superheavy elements which include both the pairing correlation and deformation by using the pairing gaps obtained from RCHB. We have thus shown that a good agreement can be obtained between theory and experimental data concerning the Q value of the α -decay. Especially, our RMF calculations reproduce a peak at $Z=114$ seen in the experimental data. We conjecture that this peak appears because of the shift of the shell structure, e.g. concerning nuclear shape, from $Z=114$ in FRDM to $Z=112$.

Finally we wish to make a few comments on open questions. We kept the pairing gap parameter once it has been fixed for a spherical shape, ignoring the possibility of its shape dependence [19]. Another basic assumption is that the observed α -decays are from ground state to ground state, though this might not be the case for a part of the α -decay chain. We noticed a paper by Cwiok et al. [20] after we have completed our study. The validity of the above mentioned approximation and assumption will be worth being examined to obtain more reliable understanding of superheavy elements. It would also be important to understand the difference between our conclusions and those in ref. [20], where the authors predict systematically much smaller deformation for all nuclei and also claim that the de-

formation monotonically decreases towards $Z=118$. We will address these questions in a separate paper.

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